

Supplementary Information for

A family of all sp^2 -bonded carbon allotropes of topological semimetals with strain-robust nodal-lines

Zhiqiang Zhao, Zhuhua Zhang* and Wanlin Guo

State Key Laboratory of Mechanics and Control of Mechanical Structures, Key Laboratory for Intelligent Nano Materials and Devices of Ministry of Education, and Institute of NanoScience, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, China

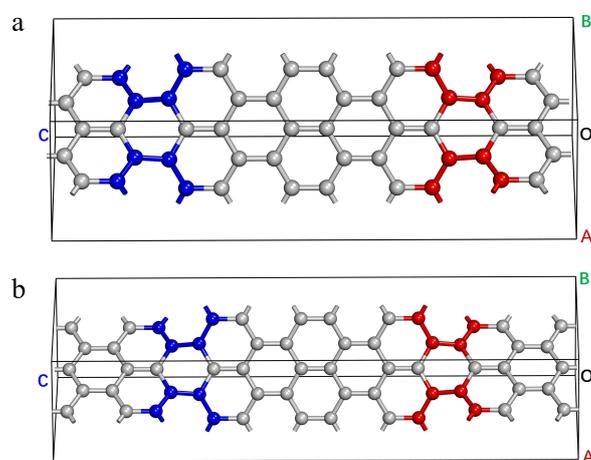


Fig. S1. Structures for *mrs*-C₄₀ and *ors*-C₄₈. (a) Perspective of *mrs*-C₄₀, containing 40 atoms in the unit cell with lattice parameters $a=4.931$ Å, $b=4.925$ Å and $c=21.118$ Å. (b) The 48-atoms unit cell of *ors*-C₄₈ with lattice parameters $a=4.925$ Å, $b=4.925$ Å and $c=25.118$ Å.

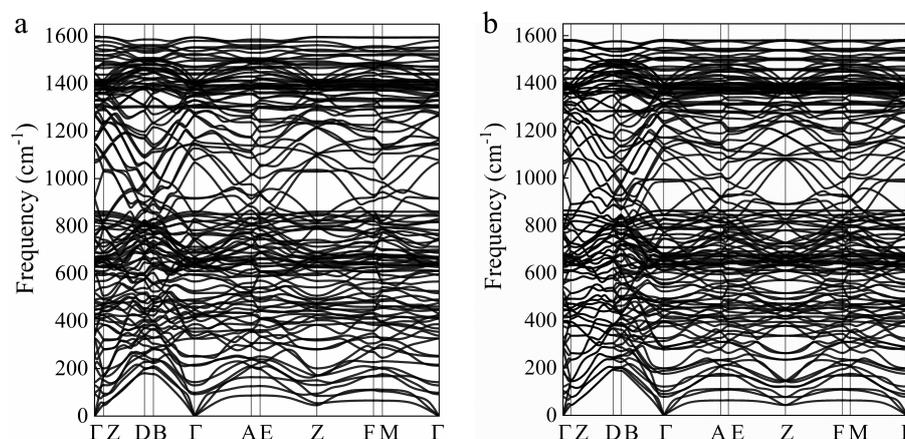


Fig. S2. Calculated phonon dispersion of *mrs*-C₄₀ (a) and *ors*-C₄₈ (b) at zero pressure.

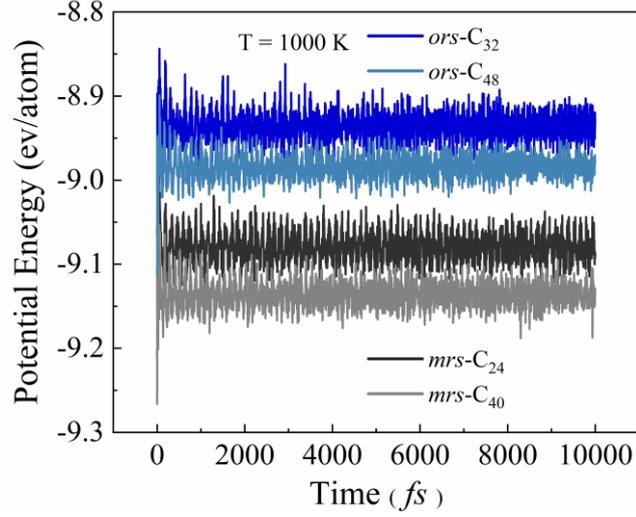


Fig. S3. Potential energy fluctuation of *mrs-C₂₄*, *ors-C₃₂*, *mrs-C₄₀* and *ors-C₄₈* in AIMD simulations at 1000 K.

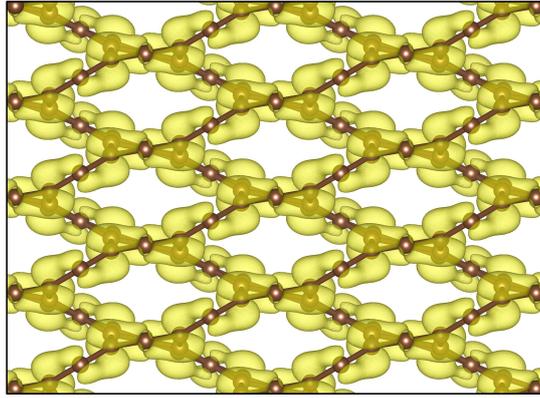


Fig. S4. Partial charge density of the highest valence band (HVB) and the lowest conduction band (LCB) near the Dirac states in the *mrs-C₂₄*, the isosurface level is $0.04 \text{ e}/\text{\AA}^3$.

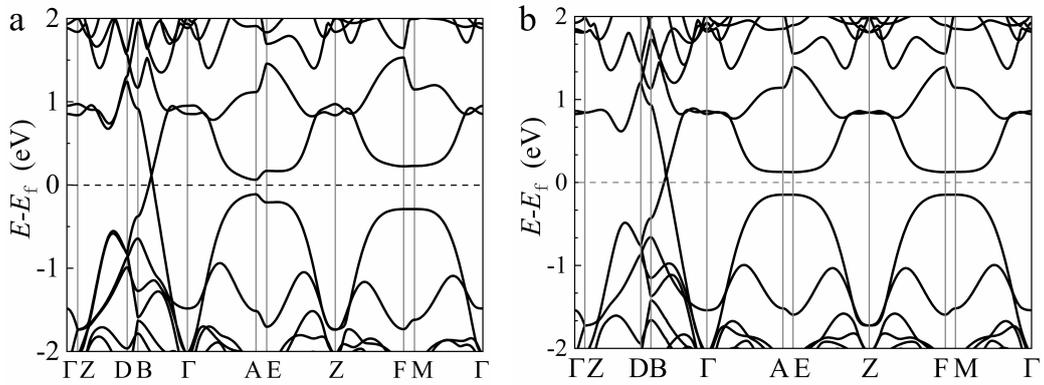


Fig. S5. Bulk band structures of *mrs-C₄₀* (a) and *ors-C₄₈* (b) along the high-symmetry pathways, which linearly cross near the Fermi level along the B- Γ path.

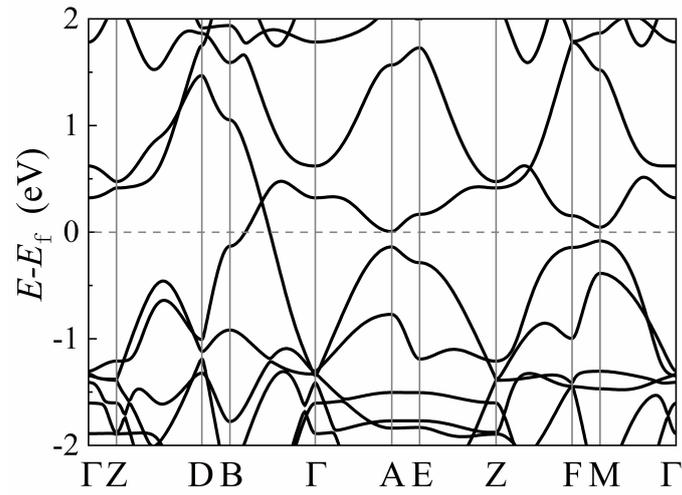


Fig. S6. Bulk band structure of the *mrs-C₄₀* along the high-symmetry pathways at a tensile strain of $\varepsilon_z=60\%$.

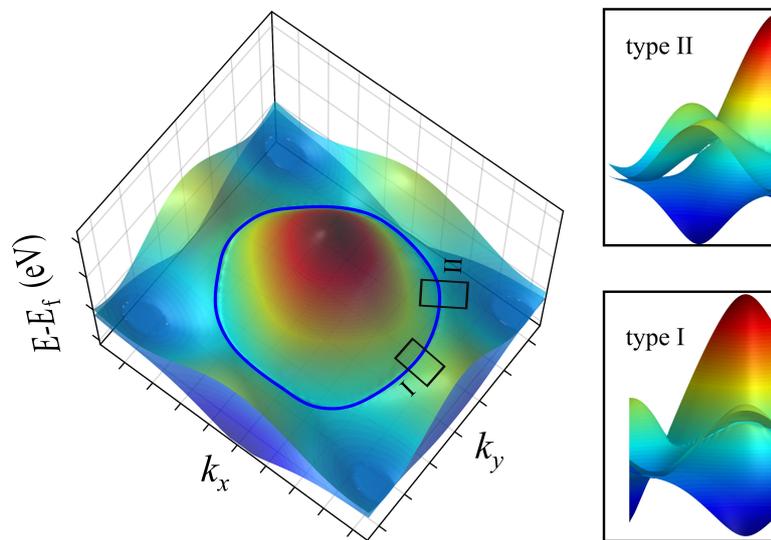


Fig. S7. 3D energy-momentum plots of the *ors-C₃₂* in low-energy states at a tensile strain of $\varepsilon_z = 65\%$. Band crossings belonging to types I and II are marked by I and II, respectively.

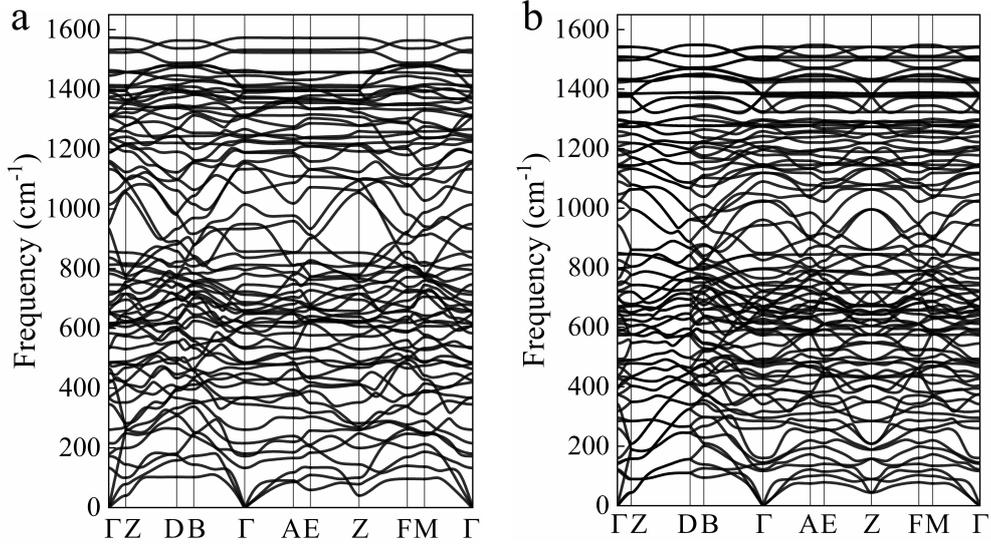


Fig. S8. Phonon band dispersions of *mrs*-C₂₄ and *ors*-C₃₂ under tensile strain. (a) The phonon dispersion of the *mrs*-C₂₄ at a tensile strain of $\epsilon_z=50\%$. (b) The phonon dispersion of the *ors*-C₃₂ at a tensile strain of $\epsilon_z=75\%$.

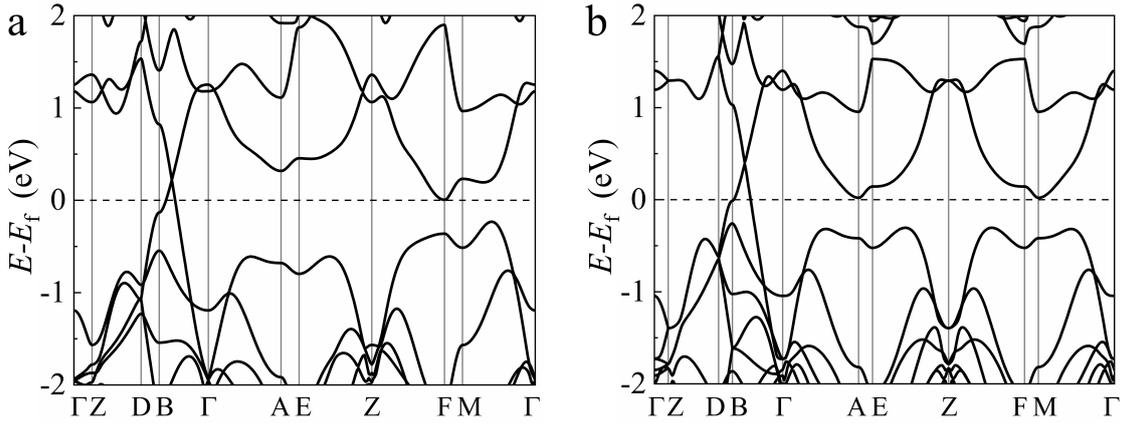


Fig. S9. Bulk band structures of *mrs*-C₂₄ and *ors*-C₃₂ under compressive strain. (a) The bulk band structure of the *mrs*-C₂₄ at a compressive strain of $\epsilon_z=3\%$. (b) The bulk band structure of the *ors*-C₃₂ at a compressive strain of $\epsilon_z=7\%$.